

10764922

FILE 'REGISTRY' ENTERED AT 18:57:18 ON 24 AUG 2004  
L1           STRUCTURE uploaded  
L2        5 S L1  
L3      167 S L1 SSS FULL  
L4           STRUCTURE uploaded  
L5        2 S L4 SUB=L3 SAMPLE  
L6      38 S L4 SSS FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 19:01:53 ON 24 AUG 2004  
L7        110 S L6  
L8        2 S L7 AND PATENT/DT  
          S L7 NOT 526-13-6/REG#

FILE 'REGISTRY' ENTERED AT 19:04:01 ON 24 AUG 2004  
L9        1 S 526-13-6/RN

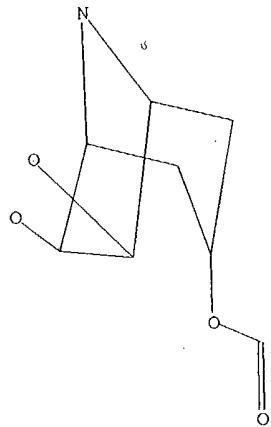
FILE 'CAPLUS' ENTERED AT 19:04:01 ON 24 AUG 2004  
L10      86 S L9  
L11     24 S L7 NOT L10  
L12     23 S L11 NOT L8  
L13           STRUCTURE uploaded  
          S L13

FILE 'REGISTRY' ENTERED AT 19:10:07 ON 24 AUG 2004  
L14      0 S L13 SUB=L3 SAMPLE

FILE 'CAPLUS' ENTERED AT 19:10:12 ON 24 AUG 2004  
L15      0 S L14 SUBSET=L3

FILE 'REGISTRY' ENTERED AT 19:10:24 ON 24 AUG 2004  
L16      0 S L13 SUB=L3 SAMPLE  
L17      0 S L13 SSS FULL SUB=L3  
L18      0 S L13  
L19      0 S L13 SSS FULL

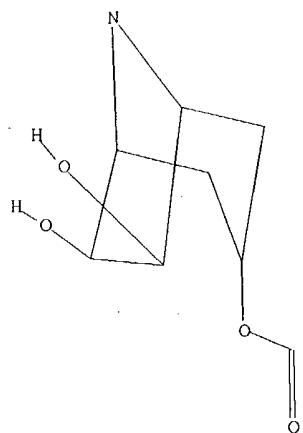
=> d 11  
L1 HAS NO ANSWERS  
L1           STR



Structure attributes must be viewed using STN Express query preparation.

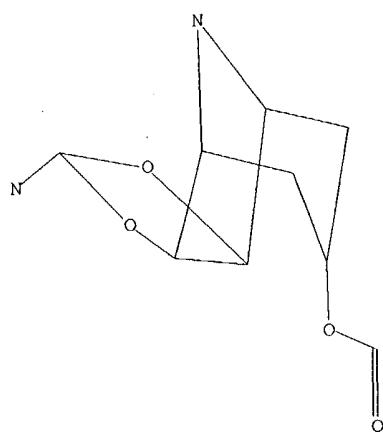
=> d 14  
L4 HAS NO ANSWERS  
L4           STR

10764922



Structure attributes must be viewed using STN Express query preparation.

=> d 113  
L13 HAS NO ANSWERS  
L13 STR



=&gt; d bib abs hitstr 1-2

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:972072 CAPLUS  
 DN 140:27968  
 TI Technical method for producing tropenol  
 IN Banholzer, Rolf; Bodenbach, Gisela; Mathes, Andreas; Meissner, Helmut;  
 Specht, Peter  
 PA Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G., Germany  
 SO PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003101986	A1	20031211	WO 2003-EP5158	20030516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10224091	A1	20031211	DE 2002-10224091	20020531
US 2003236409	A1	20031225	US 2003-448493	20030529
US 6747153	B2	20040608		
US 2004158069	A1	20040812	US 2004-764922	20040126
PRAI DE 2002-10224091	A	20020531		
US 2002-407121P	P	20020830		
US 2003-448493	A1	20030529		
OS CASREACT 140:27968; MARPAT 140:27968				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

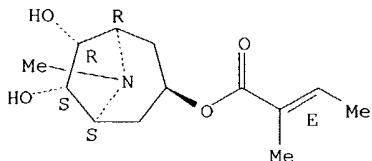
AB The invention relates to a novel, tech. applicable production method for preparing tropenol (I), optionally in the form of hydrates or acid addition salts, from tropanetriol ester II [R = C1-4-alkyl, C2-6-alkenyl, C1-4-alkylene-Ph (optionally substituted with OH or C1-4-alkoxy)] via reaction with (R'')<sub>2</sub>NCH(OR')<sub>2</sub> (R' = Me, Et; R'' = Me, Et, CH<sub>2</sub>Et), an elimination reaction of acetals III and deacylation of esters IV. Thus, tiotropium bromide was prepared from meteloidin [II; R = CMe:CHMe-(E)], via reaction with Me<sub>2</sub>NCH(OMe)<sub>2</sub>, elimination reaction of acetal III, hydrolysis of ester IV with NaOH in aqueous EtOH, transesterification by I of di(2-thienyl)glycolic acid Me ester, stereoselective epoxidn. with vanadium(V) oxide in DMF, and N-methylation with MeBr.

IT **526-13-6**, Meteloidin  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with DMF di-Me acetal; tech. method for producing tropenol)

RN 526-13-6 CAPLUS  
 CN 2-Butenoic acid, 2-methyl-, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, (2E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

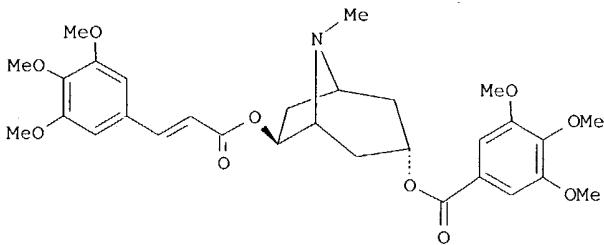


## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:814128 CAPLUS  
 DN 137:322727  
 TI Isolation of tropane alkaloid multidrug resistance inhibitors from Erythroxylum pervillei and their use for treatment of cancer and infections  
 IN Kinghorn, A. Douglas; Pezzuto, John M.  
 PA The Board of Trustees of the University of Illinois, USA  
 SO PCT Int. Appl., 108 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002083669	A1	20021024	WO 2002-US11358	20020411
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US	2003092729	A1	20030515	US 2002-119874	20020410
EP	1392685	A1	20040303	EP 2002-762037	20020411
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR	2002008791	A	20040309	BR 2002-8791	20020411
PRAI US	2001-283394P	P	20010412		
	WO 2002-US11358	W	20020411		

GI



AB The methods that utilize compds. derived from Erythroxylum pervillei and which modulate the activity of P-glycoproteins are disclosed. The compds. overcome multidrug resistance and can be used therapeutically to enhance performance of therapeutic drugs, like chemotherapeutic drug and antibiotics. Thus, new compds. pervilleine A, B (I), C, D, E, F and A N-oxide were isolated from Erythroxylum pervillei along with two known tropane alkaloid esters; they were characterized by NMR and tested for bioactivity. Pervilleine B (I) was tested for in vitro cytotoxicity against human cancer cell lines [ED<sub>50</sub> = 9.4 µg/mL (BCI); ED<sub>50</sub> = 3.1 µg/mL (Lul); ED<sub>50</sub> = 1.3 µg/mL (Col2); ED<sub>50</sub> = 0.1 µg/mL (KB-V1+); ED<sub>50</sub> = 8.8 µg/mL (KB-V1-); ED<sub>50</sub> = 1.0 µg/mL (LNCaP); ED<sub>50</sub> = 3.2 µg/mL (SW626)], multidrug resistance [IC<sub>50</sub> = 3.8 µM (SKOV3 ovarian adenocarcinoma); IC<sub>50</sub> = >10 µM (BSKVLB ovarian adenocarcinoma); IC<sub>50</sub> = 0.12 µM (SKV1B)] and the relationship of MDR-reversing activity and physicochem. properties [IC<sub>50</sub> = >35 µM (KB-3); IC<sub>50</sub> = 15 µM (KB-V); IC<sub>50</sub> = 0.17 µM (KB-V, done in the presence of vinblastine)].

IT 104086-63-7, Tropane-3 $\alpha$ ,6 $\beta$ ,7 $\beta$ -triol  
 3-phenylacetate  
 RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)  
 (isolation, NMR, crystal structure and bioactivity of; tropane alkaloid multidrug resistance inhibitors from Erythroxylum pervillei and their

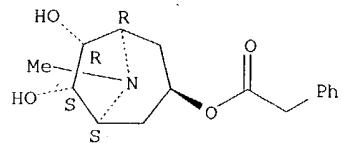
10764922

use for treatment of cancer and infections)

RN 104086-63-7 CAPLUS

CN Benzeneacetic acid, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

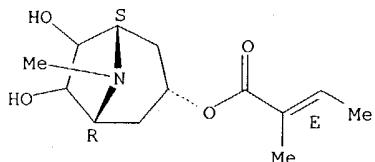
10764922

=> d 1, 5, 10, 15, 20, 23 bib abs hitstr

L12 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:716925 CAPLUS  
DN 140:108110  
TI Alkaloids of Datura ceratocaula  
AU Berkov, Strahil  
CS Department of Applied Botany, Institute of Botany, Bulgarian Academy of Sciences, Sofia, 1113, Bulg.  
SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (2003), 58(7/8), 455-458  
CODEN: ZNCBDA; ISSN: 0939-5075  
PB Verlag der Zeitschrift fuer Naturforschung  
DT Journal  
LA English  
AB Thirty-six alkaloids were identified in the organs of Datura ceratocaula by GC/MS. Thirty-three of them have not been previously reported for the species. Furthermore, a new tropane ester was tentatively identified as 3-(3'-formyloxytropoyloxy)tropane on basis of its mass spectral fragmentation. Hyoscyamine was the main alkaloid in the plant organs.  
IT 646063-97-0 646063-98-1  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(alkaloids of Datura ceratocaula)  
RN 646063-97-0 CAPLUS  
CN 2-Butenoic acid, 2-methyl-, (3-endo)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, (2E)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

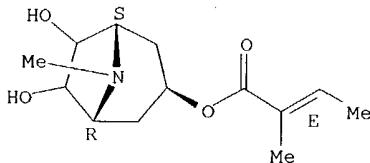
Double bond geometry as shown.



RN 646063-98-1 CAPLUS  
CN 2-Butenoic acid, 2-methyl-, (3-exo)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, (2E)- (9CI) (CA INDEX NAME)

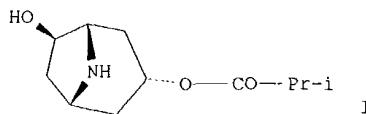
Relative stereochemistry.

Double bond geometry as shown.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:348260 CAPLUS  
DN 137:75928  
TI New tropane alkaloids from Erythroxylum moonii  
AU Khattak, Khanzadi Fatima; Atta-ur-Rahman; Choudhary, Mohammad Iqbal; Hemalal, K. D.; Tillekeratne, L. M.  
CS H.E.J. Research Institute of Chemistry, University of Karachi, International Center for Chemical Sciences, Karachi, 75270, Pak.  
SO Journal of Natural Products (2002), 65(6), 929-931  
CODEN: JNPRDF; ISSN: 0163-3864  
PB American Chemical Society  
DT Journal  
LA English  
GI



AB Four new tropane alkaloids were isolated from the leaves of *Erythroxyllum moonii* and identified as  $3\alpha$ -isobutyryloxy- $7\beta$ -hydroxynortropane (e.g. I),  $3\alpha$ -hydroxy- $7\beta$ -phenylacetoxynortropane,  $3\alpha$ -cis-cinnamoyloxytropane, and  $3\alpha$ -hydroxy-( $3'$ -hydroxy- $2'$ -methyl- $3'$ -phenylpropionyloxy)- $7\beta$ -hydroxynortropane. Other alkaloids isolated for the first time from *E. moonii* were  $3\alpha$ -benzoyloxytropane,  $3\alpha$ -phenylacetoxynortropane,  $3\alpha$ -trans-cinnamoyloxytropane, and  $3\alpha$ -phenylacetox- $6\beta$ , $7\beta$ -dihydroxynortropane. The structures of the new compds. were elucidated by spectroscopic methods.

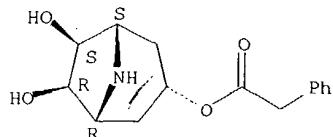
IT **439791-52-3**,  $3\alpha$ -Phenylacetox- $6\beta$ , $7\beta$ -dihydroxynortropane

RL: BSU (Biological study, unclassified); BIOL (Biological study) (tropane alkaloids from *Erythroxyllum moonii*)

RN 439791-52-3 CAPLUS

CN Benzeneacetic acid, ( $1R,3$ -endo, $5S,6S,7R$ )- $6$ , $7$ -dihydroxy- $8$ -azabicyclo[3.2.1]oct- $3$ -yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1990:175556 CAPLUS

DN 112:175556

TI Alkaloids of the genus *Erythroxyllum*. Part 10. Alkaloids of *Erythroxyllum hypericifolium* leaves

AU Al-Said, Mansour S.; Evans, William C.; Grout, Raymond J.

CS Dep. Pharm. Sci., Univ. Nottingham, Nottingham, NG7 2RD, UK

SO Phytochemistry (1989), 28(11), 3211-15

CODEN: PYTCAS; ISSN: 0031-9422

DT Journal

LA English

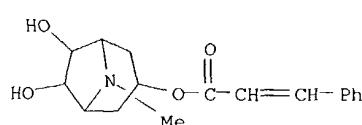
AB Fifteen alkaloids were characterized from the leaves of *E. hypericifolium*; the majority are esters of cinnamic and benzoic acids.  $3\alpha$ -Cinnamoyloxytropan- $6\beta$ -ol is the main base. New alkaloids reported are  $3\beta$ -cinnamoyloxytropane,  $3\alpha$ , $6\beta$ -dicinnamoyloxytropane,  $3$ -cinnamoyloxyntropan- $6$ -ol,  $6\beta$ -acetoxy- $3\alpha$ -cinnamoyloxytropane and, tentatively,  $6$ -phenylacetoxytropan- $3$ -ol. Two mixed cinnamate dimers were also found. Some syntheses are reported and the chemotaxonomic implications of the results are discussed.

IT **117005-30-8**

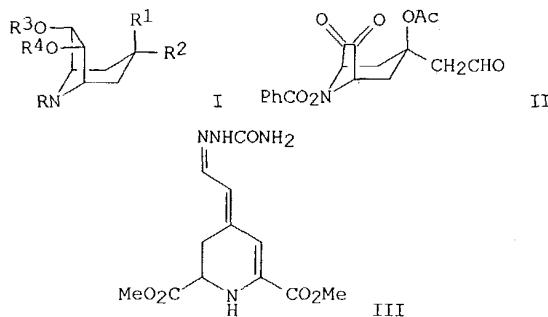
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (of *Erythroxyllum hypericifolium*)

RN 117005-30-8 CAPLUS

CN 2-Propenoic acid,  $3$ -phenyl-,  $6$ , $7$ -dihydroxy- $8$ -methyl- $8$ -azabicyclo[3.2.1]oct- $3$ -yl ester (9CI) (CA INDEX NAME)



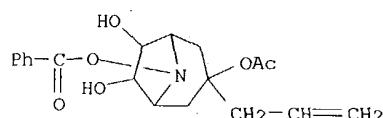
L12 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1979:39083 CAPLUS  
 DN 90:39083  
 TI Synthesis of betalains  
 AU Buchi, George; Fliri, Hans; Shapiro, Rafael  
 CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, USA  
 SO Journal of Organic Chemistry (1978), 43(25), 4765-9  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English  
 GI



AB N-Benzylnorteloidinone (I, R = PhCH<sub>2</sub>, R<sub>1</sub>R<sub>2</sub> = O, R<sub>3</sub> = R<sub>4</sub> = H), prepared by Robinson-Schopf synthesis, was converted to the ortho ester I (R = PhCH<sub>2</sub> with HC(OMe)<sub>3</sub>. Catalytic debenzylation of I (RIR<sub>2</sub> = O, R<sub>3</sub>R<sub>4</sub> = MeOCH) followed by addition of allylmagnesium bromide gave the carbinol, which was transformed to the I (R = PhCO<sub>2</sub>, R<sub>1</sub> = OH, R<sub>2</sub> = H<sub>2</sub>C:CHCH<sub>2</sub>, R<sub>3</sub>R<sub>4</sub> = MeOCH) with benzoyl peroxide. Acetylation of the tertiary carbinol was followed by hydrolysis of the ortho ester to the diol. Consecutive oxidns. of the diol to the  $\alpha$ -diketone with dimethyl sulfide-N-chlorosuccinimide, and of the olefin to the aldehyde with ozone, gave the diketo aldehyde II. Treatment of II with lead Ph(OAc)<sub>4</sub> in MeOH-C<sub>6</sub>H<sub>6</sub> gave a di-Me ester which, upon chromatog. over silica gel, lost both AcOH and BzOH to give di-Me betalamate, characterized by a crystalline semicarbazone (III) of unknown stereochem. Conversion of III to indicaxanthin and betanidin was accomplished using known procedures.

IT **63321-97-1P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 63321-97-1 CAPLUS  
 CN 8-Azabicyclo[3.2.1]octane-3,6,7-triol, 8-(benzyloxy)-3-(2-propenyl)-,  
 3-acetate, (3-endo,6-exo,7-exo)- (9CI) (CA INDEX NAME)



L12 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1972:549747 CAPLUS  
 DN 77:149747  
 TI Biosynthesis of the isovaleryl and senecioyl moieties of tropane alkaloids  
 AU Achari, R. G.; Court, W. E.; Newcombe, F.  
 CS Sch. Org. Chem., Univ. Bradford, Bradford/Yorkshire, UK  
 SO Planta Medica (1972), 22(1), 38-41  
 CODEN: PLMEA; ISSN: 0032-0943  
 DT Journal  
 LA English

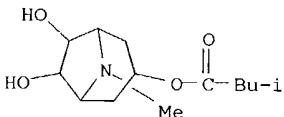
AB Incorporation of radioactivity from L-leucine-U-14C and L-valine-U-14C into 8 alkaloids extracted from *Datura sanguinea* and *D. stramonium* plants indicated that both amino acids can act as precursors to several isovaleryl and senecioyl moieties of the tropane alkaloids, including 3-senecioyl-, 3-isovaleryl-, 3,6-disenecioyl-, and 3,6-diisovaleryl esters of oxytropane; 3,6-disenecioyl- and 3,6-divalerylestes of oxytropane-7-ol, and 3-senecioyl and 3-isovaleryl- esters of oxytropane-6,7-diol.

IT **38753-89-8**

RL: BIOL (Biological study)  
(formation of isovaleryl moiety of)

RN 38753-89-8 CAPLUS

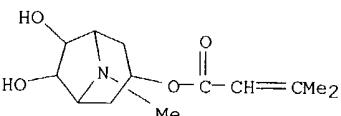
CN Butanoic acid, 3-methyl-, 6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (9CI) (CA INDEX NAME)

IT **38753-88-7**

RL: BIOL (Biological study)  
(formation of senecioyl moiety of)

RN 38753-88-7 CAPLUS

CN 2-Butenoic acid, 3-methyl-, 6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (9CI) (CA INDEX NAME)



L12 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1955:20108 CAPLUS

DN 49:20108

OREF 49:3987g-i,3988a-e

TI The synthesis of dihydrometeloidine and related compounds

AU Sheehan, John C.; Bissell, Eugene R.

CS Massachusetts Inst. of Technol., Cambridge

SO Journal of Organic Chemistry (1954), 19, 270-6

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

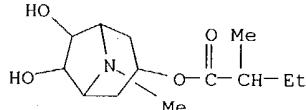
AB Dihydrometeloidine (I), structurally related to meteloidine, a natural oxygenated tropane alkaloid, has been synthesized. Teloidinone (II) (3.4 g.) and 4.2 g. p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H·H<sub>2</sub>O in 40 cc. BzH are kept 48 hrs. at 20°, ether is added, the precipitate mixed with 50 cc. N NaOH, and extracted with C<sub>6</sub>H<sub>6</sub>, giving 89% benzylideneteloidinone (III), prismatic needles, m. 150-1° [HBr salt, needles, m. 215-16° (decomposition); p-toluenesulfonate, m. 202-3° (decomposition)]. Hydrogenation of 1.95 g. III in 200 cc. 70% EtOH with W-4 Raney Ni at 20° 3-6 hrs. gives 89.5% benzylideneteloidine (IV), needles, m. 163-5° after sublimation at 120°/0.05 mm. [picrate, yellow needles, m. 189-90° (decomposition); HBr salt, m. 236-7° (decomposition)]. Adding Na to 260 mg. IV in 25 cc. liquid NH<sub>3</sub>, until the blue color persists 1 hr., decomposing the mixture with 500 mg. NH<sub>4</sub>Cl, and evaporating the NH<sub>3</sub> give 50 mg. teloidine, m. 166-8° (decomposition). Treating 1 g. IV with 6 cc. α-methylbutyric anhydride in 6 cc. C<sub>5</sub>H<sub>5</sub>N 24 hrs., concentrating the mixture in vacuo, taking up the residue in 25 cc. N HCl, extracting with ether, making the aqueous solution alkaline with 6 cc. 6N NaOH, and again extracting with ether give 61% benzylidene-α-methylbutyrylteloidine (V). HBr, platelets, m. 237.5-8.5° (decomposition) (picrate, yellow needles, m. 161-2°). Hydrogenating 500 mg. V in 10 cc. AcOH with 200 mg. prereduced 30% Pd-C at 20° gives 95.5% I, needles, m. 96-7° [HBr salt, platelets, m. 216-17° (decomposition)]. Treating 1 g. IV in 6 cc C<sub>5</sub>H<sub>5</sub>N with 4 cc. Ac<sub>2</sub>O 24 hrs. at 20° gives 80% benzylideneacetylteloidine (VI), m. 110.5-11.5° [HBr salt, needles, m. 276-7° (decomposition)]. Hydrogenolysis of 500 mg. VI gives 85% acetylteloidine (VII), m.

178.5-9.5° (decomposition) [HBr salt, m. 207-8° (decomposition)]. Acetylation of teloidine or VII with Ac 20-C5H5N at 20° gives 65% teloidine triacetate, m. 84.5-5.5°. Treating 260 mg. IV in 10 cc. ether with 220 mg. Ph2C:CO 20 hrs. at 20°, evaporating the mixture, and neutralizing the residue with HBr give 83% benzylidenediphenylacetyl teloid eine-HBr, platelets, m. 256-7° (decomposition) [methiodide, m. 205-6° (decomposition)]. Refluxing 3.4 g. II and 4.2 g. p-MeC6H4SO3H·H2O in 500 cc. Me2CO 24 hrs., adding 100 cc. 0.5N NaOH, evaporating the Me2CO, and extracting the residual solution with ether give 82.3% isopropylidene teloidinone (VIII), needles, m. 89-90° [picrate, yellow needles, m. 214-15°; HBr salt, m. 241.5-2.5°; methiodide, prisms, m. 227-8° (decomposition)]. Hydrogenation of VIII gives 94.3% isopropylidene teloidine (IX), m. 131-3° [HBr salt, needles, m. 195.5-6.5°]. Heating 215 mg. IX with 10 cc. N HCl 15 min. gives teloidine-HCl, m. 307-8° (decomposition). Isopropylidene acetyl teloideine, prepared in 77% yield in the same way as VI, prismatic needles, m. 73.5-5° [picrate, yellow needles, m. 213-14°; HCl salt, prisms, m. 289-90° (decomposition); HBr salt, needles, m. 295-6° (decomposition)]. Isopropylidene diphenylacetyl teloid eine-HBr m. 165-6.5°; methiodide, needles, m. 211-12°. Heating 215 mg. IX with 785 mg. BzCl 2 hrs. gives 38% isopropylidene benzoyl teloideine-HBr, m. 264-5° (decomposition). Refluxing 3.4 g. II and 4.2 g. p-MeC6H4SO3H·H2O in 500 cc. Me2CO, adding 100 cc. 0.5N NaOH, distilling off the Me2CO in vacuo, concentrating the aqueous solution, treating the residue with 1.5 g. NaBH4 at 20°, extracting the mixture 24 hrs. with CH2Cl2, and subliming the residue of the CH2Cl2 extract give 50% isopropylidene pseudoteloidine (X), prisms, m. 121-3° [HCl salt, m. 250-1°; HBr salt, prisms, m. 249-50° (decomposition)]. Hydrolysis of 215 mg. X 15 min. with 10 cc. N HCl gives 87% pseudoteloidine-HCl, m. 265-6° (decomposition). Isopropylidene acetyl pseudoteloidine, prepared in 83.7% yield similarly to VI, m. 125-6.5°.

IT 4074-15-1, Meteloidine, dihydro-  
(and derivs.)

RN 4074-15-1 CAPLUS  
SN 1 U 5 U T 2

CN 1 $\alpha$ H,5 $\alpha$ H-Tropane-3 $\alpha$ ,6 $\beta$ ,7 $\beta$ -triol,  
3-(2-methylbutyrate) (8CI) (CA INDEX NAME)

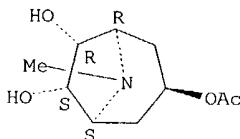


IT 109655-83-6, Teloidine, 3-acetate  
(preparation of)

RN 109655-83-6 CAPIUS

CN Teloidine, 3-acetate (6CI) (CA INDEX NAME)

## Relative stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 18:56:47 ON 24 AUG 2004)

FILE 'REGISTRY' ENTERED AT 18:57:18 ON 24 AUG 2004

L1 STRUCTURE uploaded  
L2 5 S L1  
L3 167 S L1 SSS FULL  
L4 STRUCTURE uploaded  
L5 2 S L4 SUB=L3 SAMPLE  
L6 38 S L4 SSS FULL SUB=L3

10764922

FILE 'CAPLUS' ENTERED AT 19:01:53 ON 24 AUG 2004

L7 110 S L6

L8 2 S L7 AND PATENT/DT

S L7 NOT 526-13-6/REG#

FILE 'REGISTRY' ENTERED AT 19:04:01 ON 24 AUG 2004

L9 1 S 526-13-6/RN

FILE 'CAPLUS' ENTERED AT 19:04:01 ON 24 AUG 2004

L10 86 S L9

L11 24 S L7 NOT L10

L12 23 S L11 NOT L8

=> d 2,6,11,16,21 bib abs hitstr

L12 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:297065 CAPLUS

DN 140:2784

TI Nortropane alkaloids from the leaves of Erythroxylum moonii

AU Khattak, Khanzadi Fatima; Atta-ur-Rahman; Choudhary, M. Iqbal

CS Int. Centre for Chem. Sci., H.E.J., Res. Inst. of Chem., Univ. of Karachi, Karachi, 75270, Pak.

SO Heterocycles (2003), 60(4), 917-924

CODEN: HTCYAM; ISSN: 0385-5414

PB Japan Institute of Heterocyclic Chemistry

DT Journal

LA English

AB Four new nortropane alkaloids have been isolated from the leaves of Erythroxylum moonii and identified as nortropane-3 $\alpha$ -6 $\beta$ -7 $\beta$ -triol 3-benzoate 7-(2'-hydroxy-3'-phenylpropanoate) (1), nortropane-3 $\alpha$ -7 $\beta$ -diol 7-trans-cinnamate 3-propanoate (2), nortropane-3 $\alpha$ -7 $\beta$ -diol 7-benzoate 3-(2'-methylpropanoate) (3), and nortropane-3 $\alpha$ -7 $\beta$ -diol 3-(2'-methylpropanoate) 7-cis-(3'',4'',5''-trimethoxycinnamate) (4). Addnl., five known bases are characterized as tropane-3 $\alpha$ -7 $\beta$ -diol 7-benzoate (5), tropane-3 $\alpha$ -7 $\beta$ -diol 3-phenylacetate (6), tropane-3 $\alpha$ -7 $\beta$ -diol 3-benzoate (7), tropane-3 $\alpha$ -6 $\beta$ -7 $\beta$ -triol 3-benzoate (8), and tropane-3 $\alpha$ -yl 3-(3',4',5'-trimethoxybenzoate) (9). The structures for the compds. are proposed on the basis of spectroscopic evidences.

IT 117005-29-5

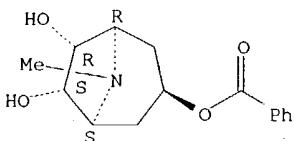
RL: NPO (Natural product occurrence); BIOL (Biological study); OCCU  
(Occurrence)

(nortropane alkaloids from leaves of Erythroxylum moonii)

RN 117005-29-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3,6,7-triol, 8-methyl-, 3-benzoate,  
(1R,3-endo,5S,6S,7R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:841082 CAPLUS

DN 136:131532

TI Modulation of the Multidrug-Resistance Phenotype by New Tropane Alkaloid Aromatic Esters from Erythroxylum pervillei

AU Silva, Gloria L.; Cui, Baoliang; Chavez, Daniel; You, Min; Chai, Hee-Byung; Rasoanaivo, Philippe; Lynn, Sean M.; O'Neill, Melanie J.; Lewis, Jane A.; Besterman, Jeffrey M.; Monks, Anne; Farnsworth, Norman R.; Cordell, Geoffrey A.; Pezzuto, John M.; Kinghorn, A. Douglas

CS Program for Collaborative Research in the Pharmaceutical Sciences and Department of Medicinal Chemistry and Pharmacognosy College of Pharmacy, University of Illinois at Chicago, Chicago, IL, 60612, USA

SO Journal of Natural Products (2001), 64(12), 1514-1520

CODEN: JNPRDF; ISSN: 0163-3864  
 PB American Chemical Society

DT Journal  
 LA English

AB Nine tropane alkaloid aromatic esters (1-9) were isolated from the roots of *Erythroxylum pervillei* by following their potential to reverse multidrug-resistance with vinblastine-resistant oral epidermoid carcinoma (KB-V1) cells. All isolates, including seven new structures (3-9), were evaluated against a panel of human cancer cell lines, and it was found that alkaloids 3 and 5-9 showed the greatest activity with KB-V1 cells assessed in the presence of vinblastine, suggesting that these new compds. are potent modulators of P-glycoprotein. Confirmatory results were obtained with human ovarian adenocarcinoma (SKV1B) cells evaluated in the presence of adriamycin and synergistic studies performed with several cell lines from the NCI tumor panel. The structures of the new compds. were determined using spectroscopic techniques. Single-crystal X-ray anal. was performed on the monoester, tropane-3 $\alpha$ ,6 $\beta$ ,7 $\beta$ -triol 3-phenylacetate (1).

IT **104086-63-7**, Tropane-3 $\alpha$ ,6 $\beta$ ,7 $\beta$ -triol

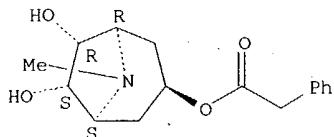
3-phenylacetate

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); BIOL (Biological study); OCCU (Occurrence)  
 (modulation of the multidrug-resistance phenotype by new tropane alkaloid aromatic esters from *Erythroxylum pervillei*)

RN 104086-63-7 CAPLUS

CN Benzeneacetic acid, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1989:404229 CAPLUS

DN 111:4229

TI Alkaloids of the genus *Erythroxylum*. Part 9. Alkaloids of *Erythroxylum hypericifolium* stem bark

AU Al-Said, Mansour S.; Evans, William C.; Grout, Raymond J.

CS Dep. Pharm. Sci., Univ. Nottingham, Nottingham, NG7 2RD, UK

SO Phytochemistry (1989), 28(2), 671-3

CODEN: PYTCAS; ISSN: 0031-9422

DT Journal

LA English

AB Thirteen bases were characterized from the stem bark of *E. hypericifolium*; hygrine is the principal component. As in the root bark esters of phenylacetic acid predominate; other alkaloids involve acetic, benzoic, and trimethoxycinnamic acids. Alkaloids reported for the first time are 3 $\alpha$ -phenylacetoxynortropan-6 $\beta$ -ol, 6 $\beta$ -acetoxy-3 $\alpha$ -benzyloxytropane, and 3-acetoxy-6-phenylacetoxytropane.

IT **104086-63-7**

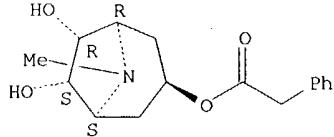
RL: BIOL (Biological study)

(from *Erythroxylum hypericifolium* stem bark)

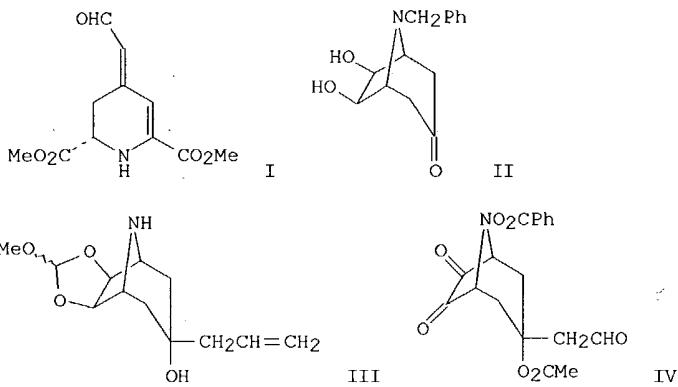
RN 104086-63-7 CAPLUS

CN Benzeneacetic acid, (1R,3-endo,5S,6S,7R)-6,7-dihydroxy-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, rel- (9CI) (CA INDEX NAME)

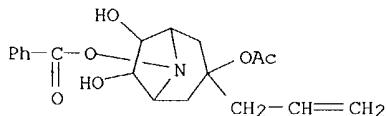
Relative stereochemistry.



L12 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1977:439714 CAPLUS  
 DN 87:39714  
 TI Synthesis of betalamic acid  
 AU Buechi, George H.; Fliri, Hans; Shapiro, Rafael  
 CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, USA  
 SO Journal of Organic Chemistry (1977), 42(12), 2192-4  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English  
 GI



AB Betalamic acid dimethyl ester (I) was prepared from N-benzylnorteloidinone (II) via the carbinol III and aldehyde IV in 9 steps.  
 IT **63321-97-1P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and oxidation of)  
 RN 63321-97-1 CAPLUS  
 CN 8-Azabicyclo[3.2.1]octane-3,6,7-triol, 8-(benzoyloxy)-3-(2-propenyl)-, 3-acetate, (3-endo,6-exo,7-exo)- (9CI) (CA INDEX NAME)



L12 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1968:484182 CAPLUS  
 DN 69:84182  
 TI Alkaloid production in Datura hybrids  
 AU Lubis, I.  
 CS Lembaga Biol. Nas., Bogor, Indonesia  
 SO Annales Bogorienses (1967), 4(3), 163-90  
 CODEN: ABOGAT; ISSN: 0517-8452  
 DT Journal  
 LA English  
 AB Alkaloid contents of the roots of Datura hybrid plants of 6 generations, produced by crossing *D. ferox* and *D. stramonium*, were determined. F-1 generation plants contained hycocamine (I) 350, hycoscine (II) 160, 3 $\alpha$ -tigloyloxytropine (III) 85, meteloidine (IV) 190, 7-hydroxy-3,6-ditigloyloxytropine (V) 400, 3,6-ditigloyloxytropine (VI) 60 mg./kg. of roots, and small amounts of tropine and an unidentified alkaloid. F-5 generation plants contained I 155, II 600, III 300, IV 355, V 200, and VI 77 mg./kg. of roots. All 6 alkaloids were detected in the roots of the

F2-F5 generation plants, but only I and II were found in the roots of F-6 plants. Unlike the case of the aerial parts of the hybrid plants, where the alkaloid characteristic of the parent D. ferox (high content of II) was dominant, the roots contained a high proportion of I up to the F-4 generation, a characteristic feature of D. stramonium. This difference was due to the inheritance of another independent genetic factor, namely the epoxidizing ability of the aerial parts, which is responsible for the formation of II from I. Variation in the amts. of III, IV, and V in the roots up to the F-5 generation indicated a tendency toward adoption of D. ferox characteristics.

IT 21631-92-5

RL: BIOL (Biological study)  
(in Datura ferox and stramonium)

RN 21631-92-5 CAPLUS

CN 1 $\alpha$ H,5 $\alpha$ H-Tropane-3 $\beta$ ,6 $\beta$ ,7 $\beta$ -triol,  
3-(2-methylcrotonate), (E)- (8CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

